Lattice-Boltzmann Simulation of Isotopic Kinetics in Crystal Growth

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RESEARCH OBJECTIVES

Isotope information in waters, sediments, and dust samples can be used to identify their sources. The relevant identification techniques utilize the isotope-ratio variations resulting from fractionation effects caused by the mass difference among the isotopes, with diffusion and reaction among the fundamental processes involved. It is especially important to know isotope behavior associated with these processes, because this determines isotope ratios and the degree of fractionation. This study is aimed at evaluating how fractionations affect the isotopic ratios in phase transformations such as evaporation, condensation, and crystal growth.

APPROACH

We used the Lattice-Boltzmann (LB) method to account for fluid flow, diffusion, and reaction in phase transformations. Isotopic kinetics were investigated by considering both diffusion and reaction rates. The effects of reaction relative to that of diffusion were described with a Damkohler number (Da).

ACCOMPLISHMENTS

LB simulations provide new insights into the behavior of isotopes when evaporation, condensation, or crystal growth occur. Results (Figure 1) show the fractionation effects for a crystal growth under different diffusion-reaction conditions. Kinetic considerations also include degree of oversaturation and the original quantity of mass to be deposited. The isotopic distributions are found to be significantly affected by the diffusive strength of the lighter and heavier isotopes in comparison with the reaction rate.

SIGNIFICANCE OF FINDINGS

LB simulation connects the crystal growth processes and isotopic kinetic effects. The simulation results explain the isotopic variation in evaporation/condensation, snow and ice formation, and crystal growth. Judging from this work, LB simulation shows potential as a method by which to evaluate the fractionation of isotopes in natural systems, extending the present simulation capability to investigate the physics bridging molecular dynamics and the conventional continuum domain.

RELATED PUBLICATIONS

Kang, Q., D. Zhang, P.C. Lichtner, and I. Tsimpanogiannis, Lattice Boltzmann model for crystal growth from supersaturated solution. J. Geophys. Res. Let., 31, L21604, 2004.

Lu, G., D.J. DePaolo, Q. Kang, and D. Zhang. Lattice Boltzmann simulation of isotopic kinetics in phase growths, J. Geophys. Res. Let. (submitted), 2005.

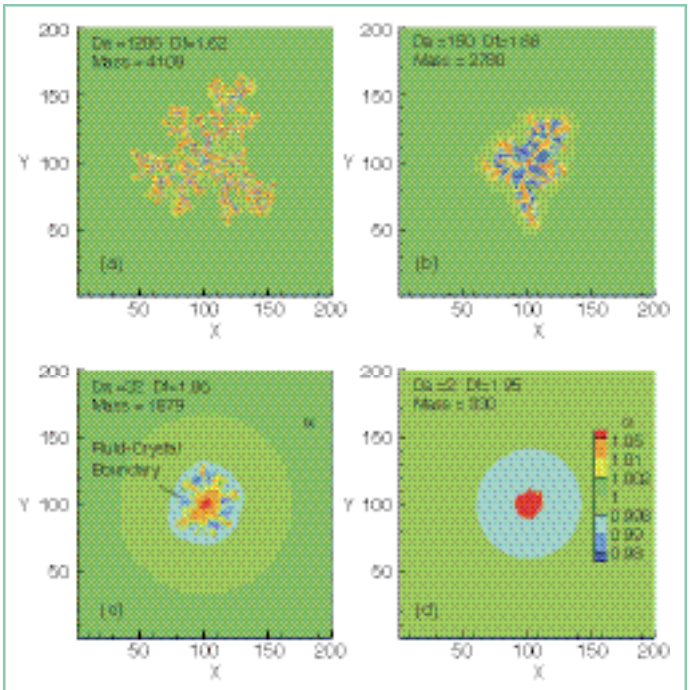

Figure 1. Calculated $^{2}H(D)/H$ isotopic fractionation effects in phase growth. Supersaturated concentration is set at 1.2, with identical reaction rate and a $^{2}H/H$ diffusion ratio of 0.972.

ACKNOWLEDGMENTS

This work was supported by Laboratory Directed Research and Development (LDRD) funding from Berkeley Lab, provided by the Director, Office of Science, of the U.S. Department of Energy under Contract No. DE-AC03-76SF0098.